

# Chemistry: Catalysis for Higher Fuel Cell Efficiency

**Objective:** Identify and evaluate catalytic surfaces aimed at improving the efficiency of Direct Methanol Fuel Cells (DMFCs).

**Implications:** Lower power, more efficient and economical DMFCs have potential applications in powering mobile phones and laptop batteries and as an alternatives to current hydrogen fuel cell technology.

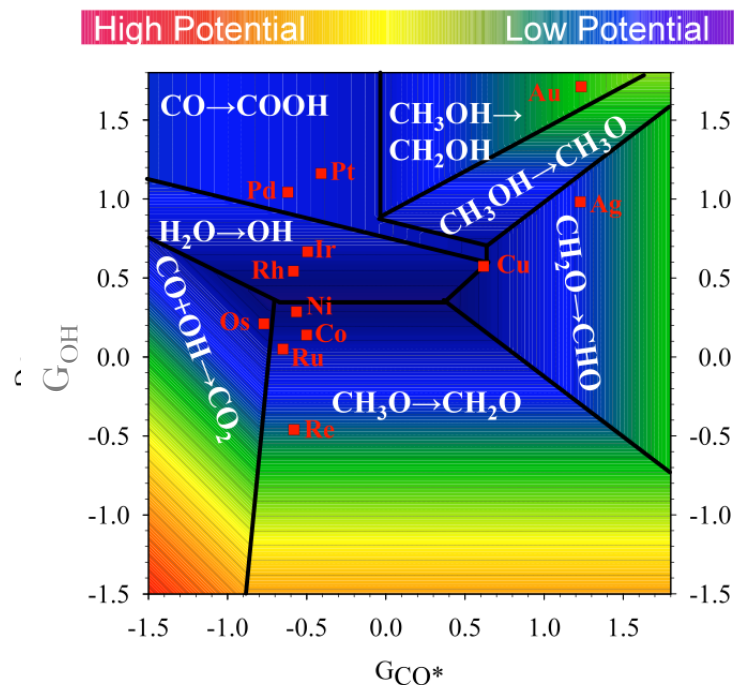
## Accomplishments:

- Used DFT to develop an electrochemical model to evaluate catalytic surfaces for methanol oxidation.
- Model helps identify properties of an 'ideal' catalyst and allows screening of novel systems that may be better and cheaper than current technology.

## NERSC:

- Used 700k hours thus far in 2009.
- Uses NERSC build of VASP application code.

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*This figure shows the potential determining steps from the DFT calculations. It helps predict the lowest possible potential of a fuel cell, which is directly related to the efficiency of the catalyst.*